

# Supporting Information

## Ultraviolet Photodepletion Spectroscopy of Dibenzo-18-Crown-6-Ether Complexes with Alkali Metal Cations

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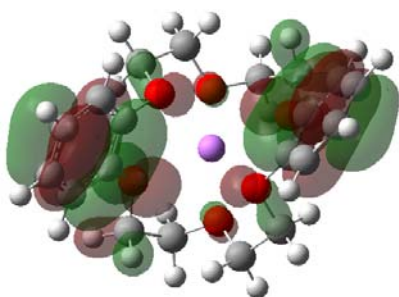
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1. Vertical singlet excitation energies in eV and oscillator strengths of  $M^+$ -DB18C6 predicted by TD-DFT at the B3LYP/6-31+G\* level of theory

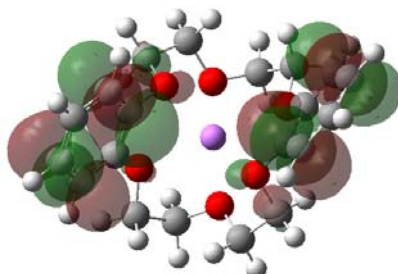
	state	main components (%)	transition energy	oscillator Strength
Cs <sup>+</sup> -DB18C6	S <sub>1</sub>	100(HOMO→LUMO)	4.7659	0.0016
	S <sub>2</sub>	100(HOMO-1→LUMO)	4.7787	0.0017
	S <sub>3</sub>	38(HOMO→LUMO+1) 34(HOMO-1→LUMO+2) 14(HOMO-3→LUMO+4)	5.0180	0.0132
Rb <sup>+</sup> -DB18C6	S <sub>1</sub>	100(HOMO→LUMO)	4.8460	0.0008
	S <sub>2</sub>	100(HOMO-1→LUMO)	4.8483	0.0053
	S <sub>3</sub>	38(HOMO-1→LUMO+1) 37(HOMO→LUMO+2) 14(HOMO-2→LUMO+4)	5.0347	0.0839
K <sup>+</sup> -DB18C6	S <sub>1</sub>	57(HOMO-1→LUMO) 22(HOMO→LUMO+1)	5.0298	0.0705
	S <sub>2</sub>	61(HOMO→LUMO) 20(HOMO-1→LUMO+1)	5.0335	0.0059
	S <sub>3</sub>	41(HOMO-1→LUMO+2) 32(HOMO-1→LUMO) 15(HOMO→LUMO+1)	5.1107	0.0116
Na <sup>+</sup> -DB18C6	S <sub>1</sub>	38(HOMO→LUMO) 34(HOMO-1→LUMO+1)	5.1074	0.0604
	S <sub>2</sub>	37(HOMO-1→LUMO) 36(HOMO→LUMO+1)	5.1092	0.0079
	S <sub>3</sub>	50(HOMO-1→LUMO) 50(HOMO→LUMO+1)	5.5408	0.0
Li <sup>+</sup> -DB18C6	S <sub>1</sub>	37(HOMO-1→LUMO) 35(HOMO→LUMO+1)	5.1502	0.0523
	S <sub>2</sub>	37(HOMO→LUMO) 34(HOMO-1→LUMO+1)	5.1519	0.0070
	S <sub>3</sub>	28(HOMO→LUMO) 25(HOMO→LUMO+1) 24(HOMO-1→LUMO+1) 22(HOMO-1→LUMO)	5.5257	0.0

## 2. Pictorial representations for HOMOs and LUMOs of $M^+$ -DB18C6

### (1) $Li^+$ -DB18C6

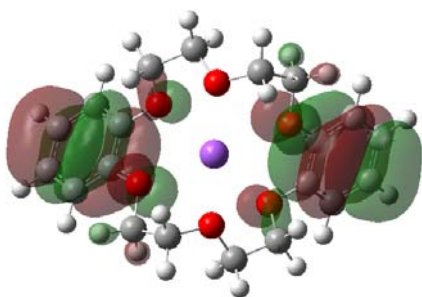


HOMO

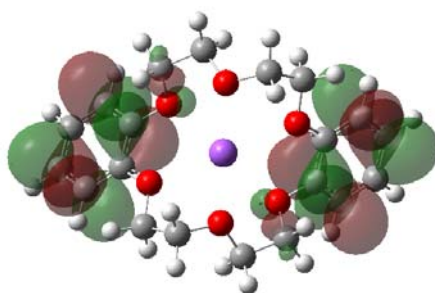


LUMO

### (2) $Na^+$ -DB18C6

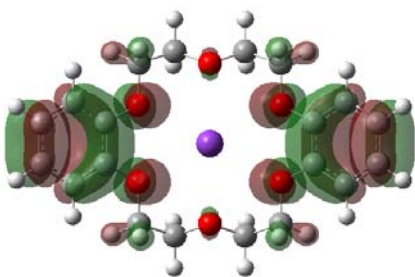


HOMO

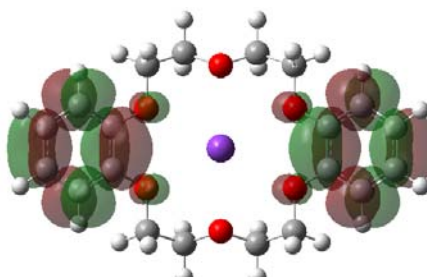


LUMO

### (3) $K^+$ -DB18C6

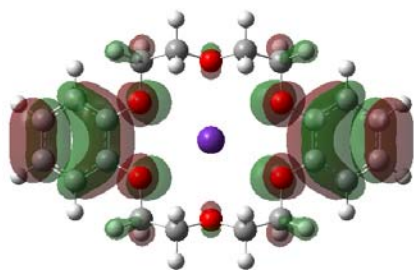


HOMO

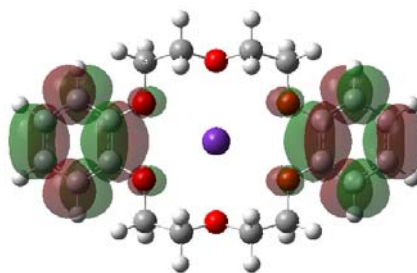


LUMO

(4)  $\text{Rb}^+$ -DB18C6

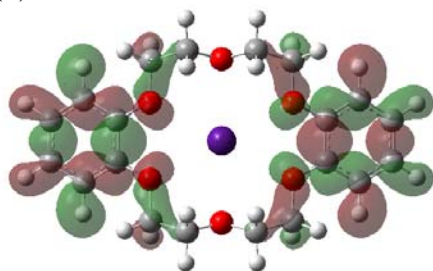


HOMO

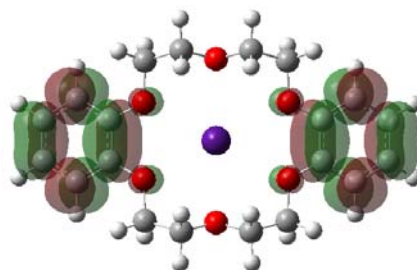


LUMO

(5)  $\text{Cs}^+$ -DB18C6



HOMO



LUMO